Abstract for oral presentation

Modelling Zinc-Air Batteries with Ionic Liquids

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The large theoretical energy density of metal-air batteries has recently stimulated a lot of research on these high-potential batteries [1],[2]. The extensive research revealed that enormous challenges lie ahead before the metal-air technology can outperform lithium ion batteries by a factor of two or three in terms of cost and energy density [3]. The key component is the electrolyte connecting the electrodes because it must be stable over a wide electrochemical window, allow reversible metal deposition, and be tolerant to air.

Ionic liquids are promising candidates for stable battery electrolytes [4]. Their advantages comprise a large electrochemical window (up to 6V), chemical and thermal stability, non-flammability (as safety asset) and low vapor pressure [5]. In particular, ionic liquids minimize dendrite growth during electrodeposition and have high ionic conductivity [5]. Zinc-air batteries with ionic liquids are potentially stable towards moisture as well as carbon dioxide and can support a reversible oxygen electrochemistry.

In this talk we present a thermodynamically consistent transport theory of zinc-air batteries based on room temperature ionic liquids. Our focus lies on the systematic derivation of a set of fully coupled transport equations for the ions, charge and heat based on the development of modeling methodologies for lithium-ion batteries [6]. Viscosity and particle nature of the medium are incorporated into the theory. Emphasis is laid on a reasonable definition for incompressibility in the context of a multi-component species. The transport theory is used to simulate the ionic liquid EmimTfo in the vicinity of an electrified interphase. We observe the two characteristic effects of crowding and overscreening. During the latter, a quasi-crystalline double layer emerges.

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